Solution of the Two-Channel Anderson Impurity Model – Implications for the Heavy Fermion UBe_{13} –

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We solve the two-channel Anderson impurity model using the Bethe-Ansatz. We determine the ground state and derive the thermodynamics, obtaining the impurity entropy and specific heat over the full range of temperature. We show that the low temperature physics is given by a line of fixed points decribing a two-channel non Fermi liquid behavior in the integral valence regime associated with moment formation as well as in the mixed valence regime where no moment forms. We discuss relevance for the theory of UBe_{13}.

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In recent years a large number of alloys have been observed to deviate from the Fermi liquid behavior, with the low temperature thermodynamics and transport physics described by logarithmic or fractional power laws. Among these are heavy fermion materials based on Ce^{3+} or U^{4+} ions containing inner shell f-electrons that do not delocalize[1]. We shall concentrate henceforth on U based materials, in particular UBe_{13}. Hund's rules and spin-orbit coupling in the presence of a cubic crystalline electric field lead to modeling of the U ion by a Γ_6 Kramers doublet in a $5f^3$ configuration to be represented by the fermionic creation operator $f_\sigma^\dagger$ and a quadrupolar (non-magnetic) doublet Γ_3 in $5f^2$ configuration represented by the operator $b_{\bar{\alpha}}^\dagger$. The doublets hybridize with conduction electrons in Γ_8 representation carrying both spin ($\sigma = \uparrow, \downarrow$) and quadrupolar ($\alpha = \pm 1$) quantum numbers. Strong Coulomb repulsion requires single occupancy of the localized levels, $f_\sigma^\dagger f_\sigma + b_{\bar{\alpha}}^\dagger b_{\bar{\alpha}} = 1$. The resulting hamiltonian is the two channel Anderson impurity model[1, 2, 3, 4, 5],

$$
\begin{aligned}
H &= H_{\text{bulk}} + H_{\text{imp}} + H_{\text{hybr}} \\
H_{\text{bulk}} &= \int \psi_{\alpha\sigma}^\dagger(x)\,(-i\partial_x)\,\psi_{\alpha\sigma}(x)\,dx \\
H_{\text{imp}} &= \varepsilon_s\, f_\sigma^\dagger f_\sigma + \varepsilon_q\, b_{\bar{\alpha}}^\dagger b_{\bar{\alpha}} \\
H_{\text{hybr}} &= V\left[\psi_{\alpha\sigma}^\dagger(0)\, b_{\bar{\alpha}}^\dagger f_\sigma + \psi_{\alpha\sigma}(0)\, f_\sigma^\dagger b_{\bar{\alpha}}\right]
\end{aligned}
$$

The spectrum is linearized around the Fermi level and the Fermi velocity is set to one with the resulting density of states being $\rho = 1/(2\pi)$. We shall study the model in the grand canonical ensemble with the chemical potential μ coupled to the total number of electrons, $N = \int \psi_{\alpha\sigma}^\dagger \psi_{\alpha\sigma}\,dx + f_\sigma^\dagger f_\sigma$. The magnetic and quadrupolar impurity doublets are at energies ε_s and ε_q respectively. The last term gives the hybridization of the host with the impurity. The bar over α indicates that the index transforms according to the conjugate representation.

The model has been intensely studied recently via a new Monte Carlo method [4] and by conserving slave boson theory [5]. However, many open questions remain. In this letter we shall present the solution of the model via a Bethe-Ansatz construction, applicable in the past only to the single channel case [6]. We shall give a complete determination of the energy spectrum and the thermodynamics, allowing us to follow the evolution of the impurity from its high temperature behavior with all four impurity states being equally populated down to the low energy dynamics characterized by a line of fixed point hamiltonians $H^*(\epsilon, \Delta)$ where $\varepsilon = \varepsilon_s - \varepsilon_q$ and $\Delta = \pi\rho V^2$ (we shall hold Δ fixed in what follows).

We shall find that the line of fixed points is characterized by a zero-temperature entropy $S_{\text{imp}}^0 = k_B \ln \sqrt{2}$ and a specific heat $C_{\text{v}}^{\text{imp}} \sim T \ln T$ typical of the 2-channel Kondo fixed point. However the physics along the line varies with ε. Consider $n_c = \left\langle f_\sigma^\dagger f_\sigma \right\rangle$, the amount of charge localized at the impurity. For $\varepsilon \lesssim \mu - \Delta$, we find $n_c \approx 1$ signaling the magnetic integral valence regime. At intermediate temperatures a magnetic moment forms which undergoes frustrated screening as the temperature is lowered, leading to zero-temperature anomalous entropy and anomalous specific heat. For $\varepsilon \gtrsim \mu + \Delta$ it is the quadrupolar integral regime and a quadrupolar moment forms. In the mixed valence regime, $|\varepsilon - \mu| \lesssim \Delta$, similar low temperature behavior is observed though without the intermediate regime of moment formation. In more detail, each point on the line of fixed points is characterized by two energy scales, $T_{l,h}(\varepsilon)$. These scales describe the quenching of the entropy as the temperature is lowered: the first stage taking place at the high temperature scale T_h, quenching the entropy from $k_B \ln 4$ to $k_B \ln 2$, the second stage at T_l, quenching it from $k_B \ln 2$ to $k_B \ln \sqrt{2}$. In the integral valence regime, $|\varepsilon - \mu| \gg \Delta$, the two scales are well separated and as long as the temperature falls between these values a moment is present, (magnetic or quadrupolar depending on the sign of $\varepsilon - \mu$), manifested by a finite temperature plateau $S_{\text{imp}} = k_B \ln 2$ in the entropy. It is quenched when the temperature is lowered below T_l, with $T_l \to T_K$ in this regime. For $\varepsilon = \mu$ the scales are equal, $T_l(\mu) = T_h(\mu)$, and the quenching occurs in a single stage. In a subsequent paper[7] we shall

present the line of boundary conformal field theories corresponding to our Bethe-Ansatz solution, and show that the two scales parameterize the approach to the fixed points.

The Bethe-Ansatz wave functions consist of plane waves with momenta $\{k_j\}$, and amplitudes that are connected by a set of scattering matrices (S-matrices) derived from the Hamiltonian and obeying Yang-Baxter consistency conditions. The electron-impurity scattering matrix is,

$$\mathbf{S}_{1,0} = \mathbf{I} - \frac{i2\Delta}{(k_1 - \varepsilon) + i2\Delta}\mathbf{Q}_{1;0}$$

where the index zero denotes the impurity. The operator $\mathbf{Q}$ acts on quadrupolar (or flavor) space as an "annihilation-creation" operator, $[\mathbf{Q}]_{\alpha;\beta}^{\alpha';\beta'} = \delta_{\alpha;\beta}\delta^{\alpha';\beta'}$. This S-matrix is unitary and group invariant. To find the electron-electron S-matrix we solve the two particle problem and find a matrix equation constraining the possible form of the S-matrix,

$$(\mathbf{S}_{2,0} - \mathbf{I})(\mathbf{S}_{1,0}\mathbf{S}_{1,2} - \mathbf{I}) = \mathbf{P}^q_{1,2}\mathbf{P}^s_{1,2}(\mathbf{S}_{1,0} - \mathbf{I})(\mathbf{S}_{2,0} - \mathbf{S}_{1,2})$$

where $\mathbf{P}^q$ is the flavor exchange operator and $\mathbf{P}^s$ the spin exchange operator, with $[\mathbf{P}^q]_{\alpha;\beta}^{\alpha';\beta'} = \delta_\alpha^{\beta'}\delta_\beta^{\alpha'}$ and similarly for $\mathbf{P}^s$. Imposing in addition the Yang-Baxter conditions, we obtain an overdetermined set of equations admitting nevertheless a unique solution:

$$\mathbf{S}_{1,2} = \frac{(k_1 - k_2) - i2\Delta\,\mathbf{P}^s_{1,2}}{(k_1 - k_2) - i2\Delta}\frac{(k_1 - k_2) + i2\Delta\,\mathbf{P}^q_{1,2}}{(k_1 - k_2) + i2\Delta}$$

The Yang-Baxter conditions and the single occupancy constraint allow the consistent generalization of the solution to an arbitrary number of electrons, N. Imposing periodic boundary conditions, one is led via standard methods to Bethe-Ansatz equations (BAE) that allow the determination of the momenta and hence the spectrum: $E = \sum_{j=1}^N k_j$. The BAE are

$$\begin{aligned}
e^{ik_jL} = \quad & \prod_{\gamma=1}^{M^s} e_1\left(k_j - \Lambda^s_\gamma\right)\prod_{\delta=1}^{M^q}[e_1\left(k_j - \Lambda^q_\delta\right)]^{-1} \\
-\prod_{\delta=1}^{M^s} \quad & e_2\left(\Lambda^s_\gamma - \Lambda^s_\delta\right) = \prod_{j=1}^{N} e_1\left(\Lambda^s_\gamma - k_j\right) \\
-\prod_{\delta=1}^{M^q} \quad & e_2\left(\Lambda^q_\gamma - \Lambda^q_\delta\right) = e_1\left(\Lambda^q_\gamma - \varepsilon\right)\prod_{j=1}^{N} e_1\left(\Lambda^q_\gamma - k_j\right)
\end{aligned}$$

where $e_n(z) = (z - in\Delta)/(z + in\Delta)$. M^s is the number of down spins and the spin-rapidities Λ^s_γ describe their dynamics. The same role is played by M^q and the flavor rapidities Λ^q_γ. The momenta $\{k_j\}$ (charge-rapidities) analogously describe the charge dynamics.

Analyzing the equations in the thermodynamic limit we find that the solutions fall into four classes: (i) real charge-rapidities; (ii) charge-spin strings: $k_\pm = \Lambda^{k,s} \pm i\Delta$; (iii) spin-strings: $\Lambda_n^{s(m_s)} = \Lambda^{\alpha(m_s)} + i\Delta\left(1 + m_s - 2n\right)$, $n = 1, \ldots, m_s$ (with arbitrary length m_s); (iv) flavor-strings: $\Lambda_n^{r(m_q)} = \Lambda^{\alpha(m_q)} + i\Delta\left(1 + m_q - 2n\right)$, $n = 1, \ldots, m_q$ (with arbitrary length m_q). A generic full-solution consists of a combination of all four kinds.

Identifying the ground state and the excitations, we sum over the latter to derive the free energy. It is expressed in terms of an infinite set of functions of the variable $\lambda = \frac{\pi}{2\Delta}(k - \mu)$. These functions, $\{\eta_b(\lambda), \eta_u(\lambda), \eta_s^n(\lambda), \eta_q^n(\lambda)\}_{n=1,\ldots,\infty}$, determine the distribution probabilities of the various excitations at temperature T (entering the equations as $\tau = \frac{\pi T}{4\Delta}$): the charge bound states, charge unbound states, spin excitations and flavor excitations, respectively. These distribution functions satisfy an infinite set of coupled non-linear integral equations: the thermodynamic Bethe Ansatz (TBA) equations,

$$\begin{aligned}
\ln\bar{\eta}_b &= -\frac{\lambda}{\tau} + G * [\mathrm{f}_{q2} - \mathrm{f}_{\bar{u}}] \\
\ln\bar{\eta}_u &= -\frac{\lambda}{2\tau} + G * [-\mathrm{f}_{\bar{b}} + \mathrm{f}_{s1} + \mathrm{f}_{q1}] \\
\ln\eta_{sn} &= G * \left[\delta_{n,1}\mathrm{f}_{\bar{u}} + \bar{\delta}_{n,1}\mathrm{f}_{sn-1} + \mathrm{f}_{sn+1}\right] \\
\ln\eta_{qn} &= G * \left[-\delta_{n,1}\mathrm{f}_{\bar{u}} - \delta_{n,2}\mathrm{f}_{\bar{b}} + \bar{\delta}_{n,1}\mathrm{f}_{qn-1} + \mathrm{f}_{qn+1}\right]
\end{aligned}$$

where we have introduced the notations $\bar{\eta} = 1/\eta$, $\mathrm{f}_\alpha = \ln(1 + \eta_\alpha)$, $\mathrm{f}_{\bar{\alpha}} = \ln(1 + \bar{\eta}_\alpha)$ and $\bar{\delta}_{n,1} = 1 - \delta_{n,1}$. The convolutions (denoted by $*$) are defined with the kernel $G(\lambda) = \frac{1}{2\pi\cosh\lambda}$. The magnetic field h_s and the quadrupolar field h_q determine the asymptotic conditions: $\lim_{n\to\infty}(K_{n+1} * \mathrm{f}_{sn} - K_n * \mathrm{f}_{sn+1}) = -2h_s/T$ and $\lim_{n\to\infty}(K_{n+1} * \mathrm{f}_{qn} - K_n * \mathrm{f}_{qn+1}) = -2h_q/T$, where $K_n(\lambda) = \frac{2n}{(2\lambda)^2 + (n\pi)^2}$.

In terms of the distribution functions, the free energy $F = F_{\mathrm{bulk}} + F_{\mathrm{imp}}$ is given by:

$$\begin{aligned}
F_{\mathrm{bulk}} &= -TL\int \rho\,\mathrm{f}_{\bar{u}}\,d\lambda - 2TL\int \rho\,\mathrm{f}_{\bar{b}}\,d\lambda \\
F_{\mathrm{imp}} &= \varepsilon_q - T\left[G * (K_1 * \mathrm{f}_{\bar{u}} + K_2 * \mathrm{f}_{\bar{b}} + \mathrm{f}_{q1})\right]_{\lambda = \frac{\pi}{J}}
\end{aligned}$$

where $J = \frac{2\Delta}{\varepsilon - \mu}$. Having solved for the distributions for given values of temperature and fields, one can compute the free energy of the impurity for any value of ε. The bulk part of the free energy is divergent and requires the introduction of a regularization scheme. On the other hand, the impurity contribution to the free energy is regular and independent of the cut-off procedure.

We turn now to study the TBA equations, considering first the zero temperature limit for which it is convenient to introduce $\xi = \tau\ln\eta$. We then have, $\lim_{\tau\to 0^+}\tau\mathrm{f} = \xi^+$ and $\lim_{\tau\to 0^+}\tau\bar{\mathrm{f}} = \xi^-$, where $2\xi^\pm = \xi \pm |\xi|$, in terms of which we are able to solve explicitly the TBA equations. We find: $\xi_b = \lambda$, $\xi_{q2} = \xi_{q2}^- = G * \xi_b^-$, $\xi_u = \xi_u^+ = \frac{\lambda}{2} - \xi_{q2}$ with all the other ξ's vanishing (the result of the convolution giving ξ_{q2} can be written down

in terms of dilogarithms). Thus in the absence of external fields, the ground state is built out of a sea of charge-spin strings filled up to $\lambda = 0$ (i.e. $k = \mu$) and a completely filled sea of 2-flavor-strings. The zero-temperature impurity level occupancy (and therefore also the charge susceptibility) can be deduced in a closed form: $n_c^0 = \int_{-\infty}^{+\infty} \frac{4(\lambda-\pi/J)\,\xi_{q2}}{[(\lambda-\pi/J)^2+\pi^2]^2}\,d\lambda$. The occupancy is integral: $n_c^0 \approx 1, 0$ for $|\varepsilon - \mu| \gg \Delta$, and non-integral elsewhere.

We turn next to study the low temperature physics, $\tau \ll 1$. In the integral valence regimes, $|\varepsilon - \mu| \gg \Delta$, $|J| \gg 1$ and the main contribution to the free energy comes from $|\lambda| \approx \pi/|J| \gg 1$. It is convenient to rewrite some equations in the TBA. Using the exact relation: $\ln \eta_b - \ln \bar{\eta}_{q1} = \lambda/\tau$, we can eliminate $\mathrm{f}_{\bar{b}}$ from the equations for $\bar{\eta}_u$ and η_{q2} and write them as: $\ln \bar{\eta}_u = -E_+^d/\tau + G * [\mathrm{f}_{s1} + \mathrm{f}_{q1}]$ and $\ln \eta_{q2} = -E_-^d/\tau + G * [\mathrm{f}_{q1} + \mathrm{f}_{q3}]$ with $E_\pm^d/\tau = G * \ln\left(1 + e^{\pm\frac{1}{\tau}(\lambda - \tau \ln \eta_{q1})}\right)$. The terms $E_\pm^d$ become driving (inhomogeneous) terms at low temperatures as $\tau \ln \eta_{q1}$ tends to zero (with τ^2 corrections). We can further approximate them as follows:

$$E_\pm^d/\tau \xrightarrow[\tau \ll 1]{} G * [\lambda/\tau]^\pm \rightarrow \begin{cases} \xrightarrow[\mp\lambda \gtrsim 1]{} e^{\pm\lambda}/\pi\tau \\ \xrightarrow[\mp\lambda \lesssim -1]{} \lambda/2\tau \end{cases}$$

Changing variables, $\zeta = \lambda - \frac{\pi}{J}$, the driving terms become, in the integral valence regime: $E_\pm^d/\tau = e^{\pm\zeta - \ln T/T_\pm}$ where $T_\pm = \frac{4\Delta}{\pi^2} e^{\pm\pi/J}$. The relation of $T_\pm$ to $T_{l,h}$ depends on the sign of $\varepsilon - \mu$ and is discussed below.

We analyze separately the magnetic and quadrupolar moment regimes. Consider first the magnetic case where $\varepsilon \ll \mu - \Delta$, and therefore $\lambda \ll -1$. In the limit of small τ, the driving term E_-^d diverges faster than E_+^d that is compensated by a decaying exponential in the numerator; thus η_{q2} tends to zero exponentially fast cutting away the equations for the higher q-flavor η's. After the identifications $\bar{\eta}_{q1} \rightarrow \eta_1^s$, $\bar{\eta}_u \rightarrow \eta_2^s$ and $\eta_{sn} \rightarrow \eta_{n+2}^s$, we recover the TBA equations of the 2–channel Kondo problem[8]. The Kondo temperature is $T_K = T_l = T_+$. (T_- is large, outside the low temperature approximation range). The identification of the resulting TBA equations in this limit with those of the 2–channel Kondo model indicates that at low temperatures, when E_-^d/τ becomes very large, the system has a localized magnetic moment. When temperature goes below T_K, overscreening will take place and in particular an entropy $S_{\mathrm{imp}} = k_B \ln\sqrt{2}$ will arise. This will also be found numerically (see below).

On the other hand, when $\varepsilon \gg \mu + \Delta$, the limit of vanishing τ drives $\bar{\eta}_u$ to zero exponentially fast and cuts away the spin η's. No remapping is required, and we recover again the TBA equations of the 2–channel Kondo model but this time for the quadrupolar degrees of freedom. The relative minus sign in the driving term reverses the 'direction of lowering temperatures' with respect to the previous case and has no further consequences. The Kondo temperature is $T_K = T_l = T_-$, below which the two spin channels will overscreen a localized quadrupolar moment.

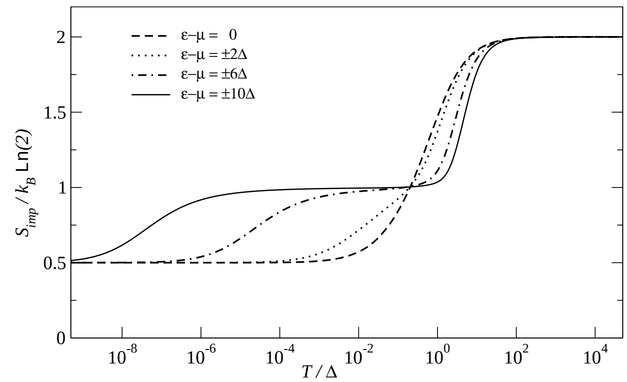

FIG. 1: Impurity contribution to the entropy as a function of temperature for different values of $\varepsilon - \mu$. As the temperature goes to zero all curves approach the universal value $k_B \ln\sqrt{2}$. Positive and negative values of $\varepsilon - \mu$ fall on top of each other.

Now we study the mixed valence regime, $|\varepsilon - \mu| \lesssim \Delta$, where $n_c \approx 1/2$. As $|J| \gg 1$, we need the solutions around $\lambda \approx 0$. Then both driving terms are approximately $E_\pm^d/\tau = e^{\pm\zeta - \ln T/T_\pm}$ and both diverge simultaneously in the low temperature limit. We repeat the standard procedure of shifting variables with $\pm \ln T/T_K$[8]. Depending on the choice of sign, one of the driving terms diverges as $1/\tau^2$ and the temperature 'disappears' from the other one. We recover one of the two cases outlined above but this time the equations are valid only at temperatures below T_l and there is no localized moment regime. However, a residual entropy $S_{\mathrm{imp}} = k_B \ln\sqrt{2}$ arises also in this regime.

Finally, we turn to the finite temperature thermodynamics. We obtain it by solving numerically the TBA equations. In Fig. 1 we show the behavior of the impurity entropy as a function of temperature for different values of ε. At high temperatures the entropy is $k_B \ln 4$ in agreement with the size of the impurity Hilbert space. For $|\varepsilon - \mu| \gg \Delta$ the impurity entropy is quenched in two stages. The degrees of freedom corresponding to the higher energy doublet are frozen first. The entropy becomes $k_B \ln 2$ and the system is in a localized magnetic or quadrupolar moment regime depending on the sign of $\varepsilon - \mu$. As the temperature is further decreased, the remaining degrees of freedom undergo frustrated screening leading to entropy $k_B \ln\sqrt{2}$. On the other hand, for values of $|\varepsilon - \mu| \ll \Delta$, the quenching process takes place in a single stage. As $\varepsilon - \mu$ is varied the behavior interpolates continuously between the magnetic and the quadrupolar scenarios. The zero temperature entropy is found to be independent of ε in accordance with the analytic study of the TBA equations. Note also the presence of a crossing point, a temperature $T_{\mathrm{cross}} \approx 0.1\Delta$ where all

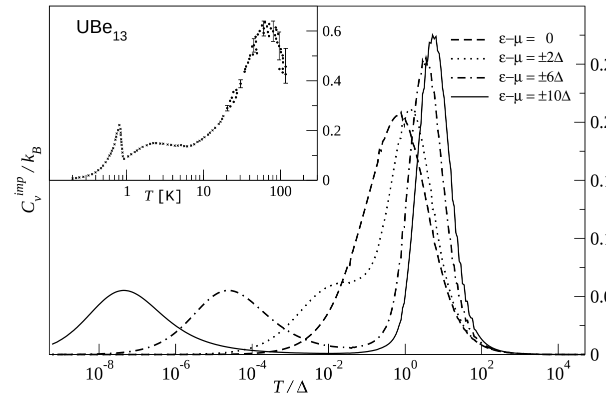

FIG. 2: Main plot: impurity contribution to the specific heat as a function of temperature for different values of $\varepsilon - \mu$. As this parameter approaches zero the Kondo contribution (left) and the Schottky anomaly (right) collapse in a single peak. Inset: experimental data for the $5f$-derived specific heat of UBe_13.

entropies take the value $S_{\rm imp} = k_B \ln 2$ independently of ε (cf. Ref. 11).

In Fig. 2 we show the impurity contribution to the specific heat. The two stage quenching process gives rise to two distinct peaks. The lower temperature peak is the Kondo contribution centered around T_l whereas the higher temperature peak often referred to as the Schottky anomaly is centered around a temperature T_h. Approximate expressions for $T_{h,l}$ can be read off from the curves: $T_{h,l}(\varepsilon) \approx \frac{\Delta}{a\pi^2} \ln(1 + 2a\, e^{\pm\frac{\pi}{2\Delta}|\varepsilon-\mu|})$ with $1 < a < 4$ (this expression goes over to $T_\pm$ defined before in the appropriate limits). For large $|\varepsilon - \mu|$ the two peaks are clearly separated and the area under the Kondo peak is $k_B \ln\sqrt{2}$ while that under the Schottky peak is $k_B \ln 2$.

As mentioned earlier, the model was proposed as a description for the U ion physics of UBe_{13}. It is expected to describe the lattice above some coherence temperature. We provide in the inset of Fig. 2 the experimental data for the $5f$-derived specific heat of the compound. It is obtained by subtracting from its total specific heat, the specific heat of the isostructural compound $ThBe_{13}$ containing no $5f$ electrons[12]. This way one is subtracting the phonon contribution as well as the electronic contribution from electrons in s, p and d shells (the procedure is quite involved and we refer the reader to the articles cited just above for full details). The sharp feature at $0.8K$ signals the superconducting transition of UBe_{13} and falls outside the range where this compound might be described by an impurity model.

Concentrating on the temperature range containing the Kondo and Schottky peaks we conclude that no values of ε and Δ yield a good fit. Further, the entropy obtained by integrating the weight under the experimental curve falls between $k_B \ln 4$ and $k_B \ln 6$. This suggests that a full description of the impurity may involve another high energy multiplet (possibly a triplet cf. Ref. 9), almost degenerate with the Γ_3 to yield a single peak for the Schottky anomaly. The nature of the multiplet could be deduced from further specific heat measurements. For an n-plet degenerate with the Γ_3, one has an $SU(2) \times SU(n+2)$ Anderson model and the area under $C_{\rm v}^{\rm imp}/T$ is then given by $k_B \ln[\frac{n+4}{2} \sec\frac{\pi}{n+4}]$, while if the n-plet is slightly split off the doublet, the area is given by $k_B \ln[\frac{n+4}{\sqrt{2}}]$ [13]. In order to be certain of having eliminated lattice effects it would be better to carry out the measurements on $U_{1-x}Th_xBe_{13}$. For $x > 0.1$ the compound has no longer a superconducting transition and the lattice coherence effects are largely suppressed. Further, there are several experimental indications that support the idea of an impurity model description of the thoriated compound for a wide range of temperatures [14].

In subsequent work we shall present the solution of the general $SU(N) \times SU(M)$ model and study the effects of magnetic and quadrupolar fields. These will help identify what particular impurity model is best fit for describing $U_{1-x}Th_xBe_{13}$ [9].

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